Edge states generated by spin-orbit coupling at domain walls in magnetic semiconductors

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Electronic states localized at domain walls between ferromagnetically ordered phases in two-dimensional electron systems are generated by moderate spin-orbit coupling. The spin carried by these states depends on the slope of the magnetic background at the domain wall. The number of localized states is determined by a real space topological number, and spin perpendicular to the ferromagnetic order accumulates in these localized states at domain walls. These trapped states may be observed in experiments that probe either spin density or conduction paths in quantum wells.

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Spin transport and spin dynamics in semiconductors have attracted considerable recent interest. Spin currents in response to an applied electric field have been found in both hole-doped semiconductors [1] and the electron-doped two-dimensional quantum well with structure inversion asymmetry in the third direction [2]. These spin currents are referred to as intrinsic spin currents in the sense that they do not depend on relaxation by impurity scattering, and the resulting "spin Hall effect" preserves time-reversal symmetry, unlike the ordinary Hall effect. However, in semiconductors such as GaAs time-reversal symmetry can be easily broken if the sample is doped with dilute Mn ions, since the Mn ions develop ferromagnetic order even at rather low doping [3, 4]. The ferromagnetic order couples to itinerant electrons or holes through both the resulting magnetic field and local "Hund's rule" coupling, and hence affects the motion of charge carriers; an example is the anomalous Hall effect measured in experiments on (Ga,Mn)As [5].

This work studies how magnetic domain formation modifies conduction electron states in magnetic semiconductors that also have spin-orbit coupling (recall that the existence of spin-orbit coupling alone does not break time-reversal). In a sample with spin-orbit coupling, the conduction electron magnetization near a domain wall (the boundary between oppositely directed domains) has a component perpendicular to the external field or the local ferromagnetic order, due to one-dimensional electronic edge states localized at the domain wall. The pair of chiral, spin-polarized electron modes at an edge can also lead to an unconventional spin-transport mechanism. The mathematical origin of these domain wall states is very similar to the origin of trapped edge states in p-wave superconductors [6] and their fractional quantum Hall analogue [7].

One possible way to detect the localized domain wall states we find is through spatial imaging of spin accumulation using Kerr rotation microscopy [8][9]. Spin accumulation changes the direction of polarization of incident light. If the incident light is polarized along $\hat{z}$ direction, the bulk spin will not rotate the polarization; only the domain wall states can induce a nonzero Kerr angle θ_K. By measuring the change of polarization of reflected light, the accumulation of perpendicular spin can be detected at the domain wall. Other possible ways to measure the domain wall states are through spin-polarized tunneling or imaging of electronic conduction paths [10].

Consider an n-doped narrow-gap semiconductor quantum well with an asymmetric confining potential in the $\hat{z}$ direction (i.e., perpendicular to the well). In this case, the conducting electron band has a Rashba spin-orbit coupling [11] term

$$H_{so} = \alpha(k_x\sigma^y - k_y\sigma^x) \tag{1}$$

In typical GaAs wells, α is about 10^{-12} eV-m [12][13], which is quite weak. However, in some materials, for instance HgTe, the Rashba coupling α is about 100 times larger than in GaAs[14][15], and since the Rashba spin-orbit coupling is linear instead of quadratic with momentum, the spin-orbit coupling will become the dominant term in the Hamiltonian as long as k is small. Furthermore, if the sample is doped with Mn ions, then time-reversal symmetry could be broken by the long-ranged order of local moments of Mn ions. Mn ions are acceptors in semiconductor, but the physics discussed here can be realized if more donators are also doped other than Mn ions. Assume for simplicity that the Mn ions develop ferromagnetic order in the $\hat{z}$ direction; there will then be Hund's-rule coupling between the local Mn ion and itinerant electrons, i.e., the local energy of an electron depends on whether its spin is parallel or antiparallel to the local moment. We neglect until the end of this paper orbital magnetic effects, as the exchange energy scale that determines the Hund's rule coupling is frequently dominant. The full Hamiltonian to quadratic order in k

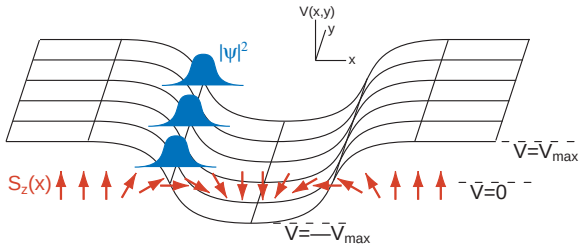

FIG. 1: The spin of localized domain wall states depends on the slope of the Zeeman field V. In this example, V is a function of x alone, and the edge state is spin-polarized along either $\hat{x}$ or $-\hat{x}$.

is then given by

$$H = \frac{k^2}{2m^*} + \alpha(k_x\sigma^y - k_y\sigma^x) + V(x)\sigma^z. \qquad (2)$$

Let us assume for the moment that the Rashba coupling is big enough to dominate the quadratic term in the Hamiltonian (2); the legitimacy of doing this will be checked later. The Hamiltonian now reads

$$H = \alpha(k_x\sigma^y - k_y\sigma^x) + V(x)\sigma^z \qquad (3)$$

If V is a constant, this is exactly the Hamiltonian for massive Dirac fermions with mass gap V. Suppose now $V(x)$ has a domain wall (a change of sign) at $x = 0$. In order to solve the spectrum of this Hamiltonian, each electron state is a spinor with components $a(x)$ and $b(x)$:

$$\psi(x,y) = e^{ik_y y}\begin{pmatrix} a(x) \\ b(x)\end{pmatrix}. \qquad (4)$$

Since k_y is a conserved quantity, the Schrödinger equation is given by

$$\begin{aligned} \alpha(-\partial_x b - k_y b) &= (E - V(x))a \\ \alpha(\partial_x a - k_y a) &= (E + V(x))b \end{aligned} \qquad (5)$$

This equation has two groups of solutions:

$$\begin{aligned} a = -b \sim e^{-\int_0^x \frac{V(x)}{\alpha}dx}, E = \alpha k_y \\ a = b \sim e^{\int_0^x \frac{V(x)}{\alpha}dx}, E = -\alpha k_y. \end{aligned} \qquad (6)$$

If $V > 0$, which means $V(x)$ is changing from negative to positive crossing the domain wall along $+\hat{x}$, only the first solution is a localized state, and it takes spin $\sigma^x = -1$, and the velocity of these states are along $+\hat{y}$. On the contrary, if $V < 0$, and $V(x)$ changes from positive to negative, the localized state is the second solution above, with velocity along $-\hat{y}$ and spin $\sigma^x = 1$. These eigenstates of the Hamiltonian indicates that there is σ^x accumulation at the domain wall, with the sign depending on the slope of the local ferromagnetic order (Fig. 1).

Note that (3) is just a Hamiltonian for massive Dirac fermions with variable mass V. That the excitation gap closes at the domain wall of V is not so surprising, but the explicit solution suggests that these massless domain wall states are chiral, with spin depending on the direction of velocity of these states. However, it is important to note that periodicity of the band structure generates an additional set of states with opposite chirality, as discussed below. The situation here is analogous to the edge states of $p \pm ip$ superconductors, in which the BdG equation breaks into two component equations [7].

So far the k^2 term has been ignored in all the calculations. When is this approximation legitimate? The term linear in k will always dominate quadratic terms when all the k involved are small. The characteristic k involved is determined by the localization length of this localized state, which is α/V. Hence the k^2 term is expected to be a small perturbation when $(V/\alpha)^2/m$ is smaller than $\alpha \times V/\alpha$, if the value of α in HgTe is taken [14][15], then V should be smaller than 10 meV, which is a typical value for magnetic semiconductors. The localization length of this state is of order 10 nm.

We now give a linear stability analysis to justify the above heuristic estimate. We have also solved model band structures for small systems to verify that trapped states indeed exist when predicted by the above intuitive criterion. Suppose that the k linear term numerically dominates the k^2 term; the stability of the localized solution for a domain wall state can be checked by solving the Schrödinger equation to linear order in $1/m$ (this linear stability is in the same spirit as the WKB method in quantum mechanics). For simplicity, $V(x)$ is taken as a step function $V(x) = V_0\mathrm{sgn}(x)$ with $V_0 > 0$. $\mathrm{sgn}(x)$ is the sign function of x, $\mathrm{sgn}(x) = +1$ when $x > 0$, and $V(x) = -1$ when $x < 0$. We assume at first order in $1/m$ that the two components of the solution of the Schrödinger equation are modified to be

$$\psi(x,y) = e^{k_y y}\begin{pmatrix} (1+f(x)/m)\exp(-\int dx\, V(x)/\alpha) \\ -(1+g(x)/m)\exp(-\int dx\, V(x)/\alpha)\end{pmatrix} \qquad (7)$$

and that the energy is slightly changed to $E = \alpha k_y + \delta E$. As long as f and g have solutions that are polynomials of x, the localized states are still stable. After solving to first order in $1/m$, f and g have the following form:

$$\begin{aligned} f(x) &= \frac{V}{\alpha^2}(k_y|x| + \frac{1}{2}\mathrm{sgn}(x)) + C \\ g(x) &= \frac{V}{\alpha^2}(k_y|x| - \frac{1}{2}\mathrm{sgn}(x)) + C \end{aligned} \qquad (8)$$

These are solutions with $\delta E = 1/m(V^2/\alpha^2 + k_y^2)$. These solutions suggest that the chiral localized states are stable even when there is a numerically small k^2 term.

The chiral domain wall localized states derived so far are not the only states localized at the domain wall, although they are the most obvious ones. Had the original model been defined on the 2d square lattice, the Rashba model would read

$$H = -t(\cos k_x + \cos k_y - 2) + \alpha(\sin k_x\sigma^y - \sin k_y\sigma^x)$$

$$+V\sigma^z. \quad (9)$$

The existence of an additional set of states is familiar from lattice simulations of chiral fermions: here, the result is an additional set of trapped states at a different momentum from the original states, as now shown.

The lattice model coefficient α has different units than in the continuum theory. If the continuum spin-orbit coupling is 10^{-12} eV-m , and the lattice constant is 10^{-10}m, the lattice model coefficient α is about 10meV. The localized states in previous paragraphs were obtained from linearizing the Hamiltonian around momentum $(0,0)$. However, the Hamiltonian (9) can always be expanded around an arbitrary momentum $\vec{k}_{0x}$ by defining the slow wave function $\tilde{\psi}(x)$ from $\psi(x) = e^{ik_{0x}x}\tilde{\psi}(x)$.

After linearizing at momentum k_{0x}, the Hamiltonian (9) becomes

$$\begin{aligned} H &= tk_x \sin k_{0x} - t\cos k_y - t(\cos k_{0x} - 2) + V\sigma^z \\ &\quad +\alpha(k_x \cos k_{0x}\sigma^y - \sin k_y \sigma^x) + \alpha \sin k_{0x}\sigma^y. \end{aligned} \quad (10)$$

Here (k_x, k_y) is the momentum of the slow mode $\tilde{\psi}$. If we ignore the last term $\alpha \sin k_{0x}\sigma^y$ first (the legitimacy will be discussed later), the resulting Schrödinger equations for the two-component spinor $\tilde{\psi} = (a,b)^T$ read

$$\begin{aligned} &-it\sin k_{0x}\partial_x a - \alpha\cos k_{0x}\partial_x b - \alpha \sin k_y b \\ &\quad = (E + t\cos k_{0x} + t\cos k_y - 2t - V)a, \\ &-it\sin k_{0x}\partial_x b + \alpha\cos k_{0x}\partial_x a - \alpha \sin k_y a \\ &\quad = (E + t\cos k_{0x} + t\cos k_y - 2t + V)b. \end{aligned} \quad (11)$$

For simplicity, assume that $V > (<)0$ when $x < (>)0$ These two equations have localized solutions as follows:

$$\begin{aligned} E &= -\frac{\sqrt{\alpha^2\cos^2 k_{0x} - t^2 \sin^2 k_{0x}}}{\cos k_{0x}} \sin k_y \\ &\quad -t\cos k_{0x} - t\cos k_y + 2t; \\ b &= \gamma a \sim \exp(\int^x dx \frac{V}{\sqrt{\alpha^2\cos^2 k_{0x} - t^2\sin^2 k_{0x}}}); \\ \langle\sigma^x\rangle &= \frac{2Re(\gamma)}{1+|\gamma|^2}, \langle\sigma^y\rangle = \frac{2Im(\gamma)}{1+|\gamma|^2}, \langle\sigma^z\rangle = \frac{1-|\gamma|^2}{1+|\gamma|^2}; \\ \gamma &= \frac{\sqrt{\alpha^2\cos^2 k_{0x} - t^2\sin^2 k_{0x}} - it\sin k_{0x}}{\alpha\cos k_{0x}}. \end{aligned} \quad (12)$$

We see for the localized states $\sin k_{0x}$ is about α/t, which is generally very small, therefore the last term in (10) is a small perturbation to the whole Hamiltonian. The stability of these localized states when k^2 and last term in (10) is taken into account can be proved in the same WKB manner as we derived formula (7).

As a check, we can assume $k_{0x} = 0$ and obtain the same answer as (6). All these localized states tend to align spin along $+\hat{x}$. These states are only localized when $\sqrt{\alpha^2\cos^2 k_{0x} - t^2\sin^2 k_{0x}}$ is a real number, which means

$$|\tan k_{0x}| < \alpha/t. \quad (13)$$

However, in order to make sure the approximate solutions in (12) are approximately orthogonal with each other, k_{0x} cannot be taken as continuous value. The intervals between each k_{0x} should be at least $2\pi V/\alpha$, which is the inverse of localization length. Therefore the total number of localized channels close to energy $E_f = 0$ is $N \approx 1 + \alpha^2/(2\pi tV)$. There are more than one localized channel if $\alpha^2/(tV) > 2\pi$, which can possibly be satisfied in systems with large spin-orbit coupling, like HgTe. States with k_{0x} within the intervals $(-\alpha/t, \alpha/t)$ and $(\pi - \alpha/t, \pi + \alpha/t)$ satisfy the condition (13), but according to the energy spectrum in (12), the states close to $k_{0x} = \pi$ have energy higher than states close to $(0,0)$ by $2t$, and the whole spectrum width of these localized states is about $2\pi\alpha$. If the Fermi energy is fixed at $E_f = 0$ and $t > \pi\alpha$, only localized states close to $k_{0x} = 0$ should be relevant. These states have the same spin alignment as in Figure. 1, but, because the energy E is a periodic function on the Brillouin zone, there is always another branch of states with velocity opposite to the ones obtained in the continuum states. The velocity is $v_y = \partial E/\partial k_y$, and since E is a periodic function of k_y, after integrating over the whole Brillouin zone the spin current $1/2\{s^x, v_y\}$ vanishes. For example, if $t = 0$, $E = -\alpha \sin k_y$, states close to $k_y = \pi$ have opposite velocity from states close to $k_y = 0$.

Many types of edge states are related to topology in momentum space [16]. Examples are the quantum Hall effect[17], and some quantum spin Hall models [18, 19, 20, 21, 22]. The usual way to bridge the bulk momentum-space topology and edge modes is through Chern-Simons theory [23], because Chern-Simons theory is gauge invariant up to a boundary term, which gives rise to chiral boson excitations at the boundary. Momentum-space topology is usually obtained in insulators, in which the whole Brillouin zone is filled; since physical quantities have the periodicity of the Brillouin zone, integrals over the whole Brillouin zone are integrals on a compact manifold, which can give rise to a nontrivial topological number. Here the situation is slightly different: there are localized domain wall modes, but the number of edge states at a single domain wall is determined by the number of bands with linear (Dirac) spectrum near the wall, which results when a band is near a minimum or maximum of the band structure neglecting spin-orbit coupling. Note that the number of domain walls is related to the number of zero crossings of the Zeeman field: to count this explicitly, a vector $\vec{N}$ has to be defined. Let the $\hat{z}$ component of $\vec{N}$ be $N_z(x) = V(x)$, and the in-plane part of the vector be $\vec{N}_{in} = \vec{\nabla}V$. The number of walls is

the Skyrmion number

$$n = \frac{1}{2\pi}\int d^2x \hat{N}\cdot(\partial_x\hat{N}\times\partial_y\hat{N}). \quad (14)$$

Here $\hat{N}$ is the unit vector along $\vec{N}$. This counting breaks down when states from different walls begin to mix. So the number of localized states is determined by this real space topological number. The spin polarization in Fig. 1 also has nonzero real space Skyrmion number, which is equal to (14).

The domain wall states affect various physical quantities. The most direct result is the σ^x magnetization. Also, once an electric field is turned on, charge current at the domain wall carries spin current (i.e., the charge current is spin-polarized), with spin maximally polarized perpendicular to the ferromagnetic order. If the width of the sample (or the length of the domain wall) L_y is shorter than the mean free length of the electrons, the modes at $k_{0x} = 0$ will induce ballistic spin current conductance similar to the weakly quantized noninteracting electric conductance in 1d systems: for voltage U, $I_s = \frac{1}{2}\frac{e}{2\pi}U$, and the total spin current conductance is obtained from summing over all the k_{0x} that satisfy (13). When $\alpha/t < 1$, the result is $Ne/4\pi$, with N the number of localized channels.

The existence of spin accumulation and spin-polarized currents can be understood from symmetry arguments. In a 2d plane with asymmetric confining potential in $\hat{z}$ as well as uniform Zeeman field $V\hat{z}$, there are the following symmetries: $\{TP_x, TP_y, P_xP_y\}$. Here P_x means $x \to -x$, P_y means $y \to -y$, and T means time-reversal. Because T, P_x and P_y all flip $V\hat{z}$, any combination of two of them should be a symmetry transformation of the system.

Therefore, spin polarization $\langle s^x\rangle$ and $\langle s^y\rangle$ are not allowed by these three symmetries. Instead, spin currents $j^x_y = 1/2\{s^x, v_y\}$ and $j^y_x = 1/2\{s^y, v_x\}$ are allowed by symmetry. However, at the domain wall along $\hat{y}$, if we assume $V(x)$ is an odd function, the symmetries are $\{P_x, TP_y\}$. Now both $\langle s^x\rangle$ and j^x_y are allowed by symmetry, consistent with the microscopic calculation given above.

For comparison to experiment, let us estimate the relative contribution to the electronic density of states from the localized states. For an estimate, suppose that the Rashba spin-orbit coupling in continuum theory is 10^{-10} eV-m (as in HgTe), the effective mass is taken as 0.1 m_e, and if V is about 10meV, there can be more than one independent localized channels at every domain wall. Then the spin density $\langle\sigma^x\rangle$ per length at the wall is about 10^8 $\hbar$ cm^{-1} times the number of channels.

We also find perpendicular spin polarization at domain walls when time-reversal symmetry of the itinerant electrons is broken by an orbital magnetic field rather than by a Zeeman field. The Hamiltonian including spin-orbit coupling for a 2D electron gas in magnetic field is

$$H = \alpha((k_x - eA_x)\sigma^y - (k_y - eA_y)\sigma^x) + B(x)g\mu_B s^z \quad (15)$$

The domain wall can be treated as the edge of two quantum Hall systems, and as is well known, the electron states at the edge are already chiral in the absence of spin-orbit coupling. The spin direction of these domain wall states can be guessed by taking the square of (15): any eigenstate of H is an eigenstate of H^2, although the converse is false. (We also ignored the quadratic term in the Hamiltonian, since the spin-orbit part will be enough for an intuitive discussion.) The square of (15) is

$$H^2 = \alpha^2(k_x^2 + (k_y - eA_y)^2) + 2eB\alpha^2\sigma^z + 2\alpha\partial_x B\mu_B s^x, \quad (16)$$

where the Landau gauge $A_x = 0, A_y = \int^x Bdx$ has been taken and $g = 2$. Far away from the domain wall, where the magnetic field is varying slowly, A_y can be taken as Bx. The first two terms are familiar to all, they are just the nonrelativistic particles moving in magnetic field. The third term results from the slope of the magnetic field, and pushes the spin along x, perpendicular to the magnetic field. Detailed calculation of the full Hamiltonian gives qualitatively the same result: spin-orbit coupling leads to confined, maximally spin-polarized edge states in the Zeeman case (which is expected to be more relevant to experiment), and also tends to spin-polarize ordinary quantum Hall edge states in the orbital case, perpendicular to the domain wall.

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